

QUANTUM GRAPHS WITH MIXED DYNAMICS: THE TRANSPORT/DIFFUSION CASE

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ABSTRACT. We introduce a class of partial differential equations on metric graphs associated with mixed evolution: on some edges we consider diffusion processes, on other ones transport phenomena. This yields a system of equations with possibly nonlocal couplings at the boundary. We provide sufficient conditions for these to be governed by a contraction semigroup on a Hilbert space naturally associated with the system. Subsequently, we devote our interest to further natural questions in the fields of parabolic and elliptic differential equations and eventually obtain a characterization of the sub-Markovian property and a description of the spectrum. We conclude the article showing that our setting is also adequate to discuss specific systems of diffusion equations with boundary delays.

1. INTRODUCTION

In the literature, usually considered problems concern networks whose ongoing dynamical processes are homogeneous: on *each* link the evolution is modeled as a transport, a diffusion, a wave, a beam, ecc. However, many physical models consist of coexisting, interacting processes of different type. On different edges a different kind of dynamics may take place; or else, one may introduce fictitious, auxiliary edges in the model in order to describe certain phenomena (like delays) in a more efficient way. Accordingly, our aim is to discuss a Cauchy problem for a system of partial differential equations of mixed type associated with an operator A : a part of the system (denoted by E_d) satisfies a one-dimensional heat equation whereas the remaining part (denoted by E_t) satisfies a one-dimensional transport equation, hence

$$A := \begin{bmatrix} \frac{d^2}{dx^2} & 0 \\ 0 & -\frac{d}{dx} \end{bmatrix}.$$

We assume the interactions of the different subsystems to take place only at the boundary. In this way we can translate our system into a vector-valued abstract Cauchy problem with suitable, non-standard coupled boundary conditions. The topic of partial differential equations on networks has become very popular in the last fifteen years, mostly due to its connections with quantum chaos which has motivated the introduction of the keyword “quantum graphs”.

As natural for a theory tightly related to mathematical physics, partial differential equations associated with observables are usually considered in the theory of quantum graphs: so far, the large majority of investigations have been devoted to self-adjoint Laplacians and other second order elliptic operators. We mention the comprehensive survey [16]. On the other hand, also some ten years ago some pioneering investigations on system of transport equations on metric graphs have been commenced in [15]. The study of the first derivative on metric graphs inside the mathematical physical community dwells on the interpretation of $i\frac{d}{dx}$ as the momentum operator, and is much less common: we are only aware of [14, 11], where some of the results of [15, 9] have been re-discovered and complemented by thorough spectral investigations. The aim of this note is to connect these two theories. The easiest case of the coupling of *one* diffusion and *one* transport equation (both possibly vector-valued) has been considered already in [12]. The work by Gastaldi and Quarteroni is presented by the authors as a first step towards the coupling of a Euler and a Navier-Stokes equation. A related viscosity analysis has been performed in [4].

In [12], well-posedness of the problem has been studied by means of viscosity methods under certain (relatively strict) coercivity assumptions. We are going to weaken the coercivity assumptions and study

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a general system consisting of finitely many coupled intervals of either type. We are going to do so by considering a large class of coupled boundary conditions for operator matrices including both second and first derivatives.

While the proposed dynamics actually seems to reflect the observed phenomena, it is very difficult to make an educated guess when it comes to propose *natural* transmission conditions. It seems that the search for correct transmission conditions, which is easy in the case of purely diffusive ([17]) or pure transport-like systems ([15]), is much less trivial in the mixed case. As Gastaldi and Quarteroni put it in [12, § 1], “When coupling Euler and Navier-Stokes equations, the proper interface conditions are not obvious, in advance. A possible way of deducing them is to see the coupled problem as a limit of two coupled Navier-Stokes problems with vanishing viscous terms [in either one of the regions]”. But even this limiting process is quite delicate, as the analysis in [12, 4] shows.

In fact our main result, Theorem 4, states that systems of the kind discussed above are well-posed under a large class of transmission conditions. Thus, we complement a spectral analysis of the considered system by the study of typical features of semigroups for heat and transport equations, in particular dissipativity and positivity. This may hopefully suggest suitable conditions in specific settings, by allowing to reject large subclasses of boundary conditions as unfit. On the other hand, while many dissipative or dispersive extensions of A can actually be found, we are not sure that one can expect contractivity or positivity of the associated semigroup, when one thinks of some motivating systems.

The plan of our article is as follows: In Section 2 we introduce the specific class of boundary conditions we are going to investigate. We discuss sufficient conditions in dependence of the boundary condition for well-posedness of the problem in the L^2 -setting and then in a general L^p -setting, while in Section 3 our attention is devoted to the positivity properties of the solutions (observe that the space of L^p -functions on a graph is a Banach lattice). In Section 4 we derive a secular equation for our system.

Unlike in [12], a possible motivation for the introduction of our setting arises from some biomathematical considerations. More precisely, it is known that electric signal coming from a neuron undergoes a certain synaptic delay before reaching another neuron, and cannot double back: this suggests to model this process by a system of diffusion (in the dendrites or axons) and transport (in the synapse) equations. In fact, it turns out that our setting can be adapted to discuss certain classes of coupled system of diffusion equations with boundary delays. This is explained in some detail in the conclusive Section 5.

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2. BOUNDARY CONDITIONS FOR A MIXED OPERATOR ON A METRIC GRAPH

We use the standard construction for the singular manifold on which the dynamic of the system is going to take place: We consider finitely many intervals of finite length that are connected to realize a simple finite metric graph G with node set V and edge set E . For the purposes of this note it is important to consider a partition of E in two disjoint subsets E_d, E_t , which are going to represent the edges on which *diffusion* and *transport* phenomena are going to take place, respectively. Hence, we denote by e_{d1}, \dots, e_{dD} and e_{t1}, \dots, e_{tT} the edges of the metric graph. To each edge e_{di} or e_{tj} we associate a length a_{di} or a_{tj} , respectively, which in turn determines an orientation of each edge from 0 to the other endpoint. More specifically, this orientation leads to the representation

$$e = \overrightarrow{(v, w)}, \quad \text{for } v, w \in V,$$

and in this case we write $e(0) = v$, $e(a) = w$. (Here and in the following a denotes the generic length – that is, either a_{di} or a_{tj} , depending on the context.)

The structure of the network is given by the $|V| \times |E|$ -*outgoing* and *ingoing incidence matrices* $\mathcal{I}^+ := (\iota_{ve}^+)$ and $\mathcal{I}^- := (\iota_{ve}^-)$ defined by

$$(1) \quad \iota_{ve}^+ : \begin{cases} 1, & \text{if } e(0) = v, \\ 0, & \text{otherwise,} \end{cases} \quad \text{and} \quad \iota_{ve}^- : \begin{cases} 1, & \text{if } e(a) = v, \\ 0, & \text{otherwise.} \end{cases}$$

The matrix $\mathcal{I} := (\iota_{ve})$ defined by $\mathcal{I} := \mathcal{I}^+ - \mathcal{I}^-$ is the incidence matrix of \mathbf{G} . Furthermore, let $\Gamma(v)$ be the set of all edges incident in v , i.e.,

$$\Gamma(v) := \{e \in E : e(0) = v \text{ or } e(1) = v\}.$$

For the sake of notational simplicity, if $e = \overrightarrow{(v, w)}$ we denote the value of a function $u_e : [0, a] \rightarrow \mathbb{C}$ on e at 0 and a by $u_e(v)$ and $u_e(w)$, respectively. With an abuse of notation, we also set $u_e(v) = 0$ whenever $e \notin \Gamma(v)$. By assumption, E is a finite measure space. The space $L^2(E)$ of square integrable functions defined on the intervals associated with the edges in E becomes a Hilbert space with respect to the natural scalar product

$$\langle u, v \rangle := \int_E u \bar{v} := \sum_{i=1}^D \int_0^{a_{di}} u_{e_{di}}(s) \overline{v_{e_{di}}(s)} ds + \sum_{j=1}^T \int_0^{a_{tj}} u_{e_{tj}}(s) \overline{v_{e_{tj}}(s)} ds.$$

By $L^2(E_d)$ and $L^2(E_t)$ we denote the $L^2(E)$ -functions with support on the edges belonging to E_d and E_t , respectively. Finally, by $H^1(E)$ we denote the Hilbert space of square integrable functions that are weakly differentiable with weak derivatives in $L^2(E)$; and use the notation $H^1(E_d) := H^1(E) \cap L^2(E_d)$ and $H^1(E_t) := H^1(E) \cap L^2(E_t)$.

On $L^2(E)$ one considers the diagonal operator matrix

$$(2) \quad A := \begin{bmatrix} \frac{d^2}{dx^2} & 0 \\ 0 & -\frac{d}{dx} \end{bmatrix}, \quad \text{i.e.,} \quad Au := A \begin{bmatrix} u_d \\ u_t \end{bmatrix} := \begin{bmatrix} u_d'' \\ -u_t' \end{bmatrix}.$$

We are going to present a class of m -dissipative realizations of A with domains containing the minimal one $H_0^2(E_d) \oplus H_0^1(E_t)$ and contained in the maximal one $H^2(E_d) \oplus H^1(E_t)$: that these are the extreme relevant cases follows from the observation that in both cases the transport and the diffusion part are clearly edge-wise decoupled.

Remark 1. *It has been observed in [16] that the most general class of self-adjoint extensions of the second derivative acting on the space of L^2 -functions over a metric graph with m edges (each identified with an interval $(0, 1)$) can be parametrized by a family of boundary conditions*

$$(3) \quad P^\perp \begin{bmatrix} -u'(0) \\ u'(1) \end{bmatrix} + (L + P) \begin{bmatrix} u(0) \\ u(1) \end{bmatrix} = 0,$$

where P is any orthogonal projection of \mathbb{C}^{2m} and L is any Hermitian matrix that can be seen as an operator on the range of $P^\perp := \mathbf{1} - P$. (This kind of coupled conditions had already appeared in [7] in an investigation of Sturm–Liouville problems on graphs). Moreover, it has been implicitly observed in [9] that the first derivative acting again on $L^2(0, 1)^m$

$$(4) \quad u(1) = Uu(0)$$

generates a unitary group (i.e., by Stone's theorem, $i \frac{d}{dx}$ is a self-adjoint operator on $L^2(0, 1)^m$) if and only if U is a unitary $m \times m$ -matrix. When one tries to couple first and second derivatives by their boundary values, one soon observes that conditions of the form (4), while strongly motivated by the integration by parts formula, are not easily related to (3) – which in turn arise from the Gauß–Green formulae. A possible way to overcome this problem is to write (4) as

$$(5) \quad |u(1)|^2 = |Uu(0)|^2 \quad \text{or rather} \quad \operatorname{Re} \langle u(1) + Uu(0), u(1) - Uu(0) \rangle = 0.$$

We impose conditions that force the numerical range into the complex left half-plane. An elementary integration by parts yields

$$(6) \quad \begin{aligned} \langle Au, v \rangle &= \int_{E_d} \langle u_d'', v_d \rangle - \int_{E_t} \langle u_t', v_t \rangle \\ &= - \int_{E_d} \langle u_d', v_d' \rangle + [u_d', v_d]_{\partial E_d} + \int_{E_t} \langle u_t, v_t' \rangle - [u_t, v_t]_{\partial E_t}, \end{aligned}$$

for $u, v \in H^2(\mathbb{E}_d) \oplus H^1(\mathbb{E}_t)$, where here and in the following we denote

$$\begin{aligned} [u_d, v_d]_{\partial \mathbb{E}_d} &:= \sum_{i=1}^D (u_{di}(a_{di}) \overline{v_{di}}(a_{di}) - u_{di}(0) \overline{v_{di}}(0)), \\ [u_t, v_t]_{\partial \mathbb{E}_t} &:= \sum_{j=1}^T (u_{ti}(a_{tj}) \overline{v_{tj}}(a_{tj}) - u_{ti}(0) \overline{v_{tj}}(0)) \end{aligned}$$

and for brevity $|u_t|_{\partial \mathbb{E}_t}^2 := [u_t, u_t]_{\partial \mathbb{E}_t}$. While the equation (6) is not particularly appealing, the real part of the associated form is

$$(7) \quad \operatorname{Re} \langle Au, u \rangle = - \int_{\mathbb{E}_d} |u'_d|^2 + \operatorname{Re}[u'_d, u_d]_{\partial \mathbb{E}_d} - \frac{1}{2} |u_t|_{\partial \mathbb{E}_t}^2, \quad u \in H^2(\mathbb{E}_d) \times H^1(\mathbb{E}_t).$$

For the sake of notational simplicity we introduce the $2|\mathbb{E}_d| + |\mathbb{E}_t|$ dimensional (“boundary”) Hilbert space

$$\mathcal{H} = \mathcal{H}_d^+ \oplus \mathcal{H}_d^- \oplus \mathcal{H}_t, \quad \mathcal{H}_d^\pm := \mathbb{C}^{|\mathbb{E}_d|}, \quad \mathcal{H}_t := \mathbb{C}^{|\mathbb{E}_t|}$$

and define for all $u \in H^2(\mathbb{E}_d) \times H^1(\mathbb{E}_t)$ the two vectors $\underline{u}, \underline{\underline{u}} \in \mathcal{H}$, where

$$(8) \quad \underline{u} := \begin{bmatrix} \{u_{di}(a_{di})\}_{1 \leq i \leq D} \\ \{u_{di}(0)\}_{1 \leq i \leq D} \\ 2^{-\frac{1}{2}} \{u_{tj}(a_{tj}) + u_{tj}(0)\}_{1 \leq j \leq T} \end{bmatrix} \quad \text{and} \quad \underline{\underline{u}} := \begin{bmatrix} \{u'_{di}(a_{di})\}_{1 \leq i \leq D} \\ \{-u'_{di}(0)\}_{1 \leq i \leq D} \\ 2^{-\frac{1}{2}} \{-u_{tj}(a_{tj}) + u_{tj}(0)\}_{1 \leq j \leq T} \end{bmatrix}$$

are given with respect to the decomposition of \mathcal{H} . With this notation, equation (7) becomes

$$(9) \quad \operatorname{Re} \langle Au, u \rangle = - \int_{\mathbb{E}_d} |u'_d|^2 + \operatorname{Re} \langle \underline{u}, \underline{\underline{u}} \rangle_{\mathcal{H}} \quad u \in H^2(\mathbb{E}_d) \times H^1(\mathbb{E}_t).$$

These computations motivates us to introduce a class of boundary conditions of the form

$$(10) \quad P^\perp \underline{u} + (L + P) \underline{u} = 0,$$

where P is an orthogonal projector acting in \mathcal{H} , $P^\perp := \operatorname{Id} - P$ denotes the complementary orthogonal projector and the matrix L is an operator in the subspace $\operatorname{Ker} P \subset \mathcal{H}$ (whose extension by 0 to the whole of \mathcal{H} we still denote by L). The boundary conditions can be equivalently written as

$$P^\perp \underline{u} + L \underline{u} = 0 \quad \text{and} \quad P \underline{u} = 0.$$

Finally we define the operator $A_{P,L}$ which is studied in this work to be given by $A_{P,L} u := Au$ on the domain

$$D(A_{P,L}) := \{u \in H^2(\mathbb{E}_d) \times H^1(\mathbb{E}_t) \mid P^\perp \underline{u} + (L + P) \underline{u} = 0\}.$$

Remark 2. We call the boundary conditions (10) type-decoupling if

- P is an orthogonal projection of $L^2(\mathbb{E})$ onto $\{0\}$, \mathcal{H} , $\mathbb{C}^{2|\mathbb{E}_d|} \times \{0\}$, or $\{0\} \times \mathbb{C}^{|\mathbb{E}_t|}$, and additionally
- L is a block-diagonal matrix with respect to the decomposition $\mathcal{H} = \mathbb{C}^{2|\mathbb{E}_d|} \oplus \mathbb{C}^{|\mathbb{E}_t|}$.

In other words, the boundary conditions are type-decoupling if actually no interaction between the boundary values in $L^2(\mathbb{E}_d)$ and $L^2(\mathbb{E}_t)$ takes place: this is of course the most trivial case, because the dynamics of the system can be effectively reduced to that of two distinct, non-interacting systems – a diffusive one and a transport one.

Lemma 3. The vector space $H^1(\mathbb{E}) := H^1(\mathbb{E}_d) \oplus H^1(\mathbb{E}_t)$ is a Hilbert space with respect to the natural inner product

$$\langle u, v \rangle_{H^1(\mathbb{E})} := \langle u', v' \rangle_{L^2(\mathbb{E}_d)} + \langle u', v' \rangle_{L^2(\mathbb{E}_t)} + \langle u, v \rangle_{L^2(\mathbb{E})}.$$

The same holds for $\{u \in H^1(\mathbb{E}) : u_d \in H^2(\mathbb{E}_d)\} = H^2(\mathbb{E}_d) \oplus H^1(\mathbb{E}_t)$ with the inner product

$$\langle u'', v'' \rangle_{L^2(\mathbb{E}_d)} + \langle u, v \rangle_{H^1(\mathbb{E})}.$$

Their embedding into $L^2(\mathbb{E})$ is dense and of p -th Schatten class for all $p > 1$. Furthermore, there exists $C > 0$ such that the Gagliardo–Nirenberg-type estimate

$$(11) \quad \|u\|_{L^\infty(\mathbb{E})}^2 \leq C \|u\|_{L^2(\mathbb{E})} \|u'\|_{L^2(\mathbb{E})} \quad \text{for all } u \in H^1(\mathbb{E})$$

holds.

Proof. Throughout this note we are assuming our graph to be compact, hence the embedding of $H^2(\mathbf{E}_d) \oplus H^1(\mathbf{E}_t)$ into $L^2(\mathbf{E}_d) \oplus L^2(\mathbf{E}_t)$ is of p -th Schatten class for all $p > 1$, cf. [13].

A constant $C > 0$ can always be found so that (11) holds, as this inequality can be reduced the case of intervals. Let namely $u \in H^1(0, 1)$, then

$$(12) \quad |u(1)|^2 \leq 2\sqrt{2}\|u\|_{L^2(0,1)}\|u\|_{H^1(0,1)}.$$

Indeed if $u \in H^1(0, 1)$ is such that $u(0) = 0$, we can write

$$|u(y)|^2 \leq \int_0^1 (u^2)'(x) dx \quad \text{for all } y \in [0, 1],$$

and by Cauchy-Schwarz's inequality we get

$$|u(y)|^2 \leq 2\|u\|_{L^2(0,1)}\|u'\|_{L^2(0,1)} \quad \text{for all } y \in [0, 1].$$

For a general $u \in H^1(0, a)$, it suffices to apply the previous estimate to $u(x) = (1 - \frac{x}{a})u(\frac{x}{a}) + \frac{x}{a}u(\frac{x}{a})$. To derive (11) on the whole graph it suffices to sum up the estimates obtained on each edge separately. \square

We are finally in the position to state our main result.

Theorem 4. *Let be P an orthogonal projector acting on \mathcal{H} and L a linear operator on $\text{Ker}P$. Then the operator $A_{P,L}$ is quasi- m -dissipative. It is even m -dissipative whenever $-L$ is dissipative. Accordingly, $A_{P,L}$ generates a quasi-contractive (contractive, if $-L$ is dissipative) semigroup on $L^2(\mathbf{E})$.*

Of course, the semigroup generated by $A_{P,L}$ is reducible (i.e., it leaves some non-trivial ideal of $L^2(\mathbf{E})$ invariant: in this case, some function space over a subset of \mathbf{E}_d or \mathbf{E}_t) if the boundary conditions (10) are type-decoupling in the sense of Remark 2.

Before proving this theorem, we need two preparatory lemmata.

Lemma 5. *Let $\omega \geq 0$ be such that $-L - \omega$ is dissipative. Then*

$$\text{Re}\langle A_{P,L}u, u \rangle \leq \frac{\omega^2 C^2}{4}\|u\|_{L^2(\mathbf{E})}^2 \quad \text{for } u \text{ all satisfying (10) } u \in D(A_{P,L}),$$

where $C > 0$ is a constant, depending only on the total length of the graph, such that

$$(13) \quad |\underline{u}|^2 \leq C\|u\|_{L^2(\mathbf{E})}\|u'\|_{L^2(\mathbf{E})} \quad \text{for all } u \in H^1(\mathbf{E}).$$

Of course, such an ω always exists: simply take $\omega := \|L\|$, although this is in general not optimal.

Proof. Take $u \in D(A_{P,L})$. Then it follows from (9) that

$$-\text{Re}\langle A_{P,L}u, u \rangle = \|u'\|_{L^2(\mathbf{E}_d)}^2 + \text{Re}\langle L\underline{u}, \underline{u} \rangle_{\mathcal{H}}.$$

If $-L$ is dissipative, then we just estimate this by

$$-\text{Re}\langle A_{P,L}u, u \rangle \geq \|u'\|_{L^2(\mathbf{E})}^2 \geq 0.$$

If instead $-L$ is only quasi-dissipative, i.e., if $-L - \omega$ is dissipative, then we deduce that for all $\epsilon > 0$

$$(14) \quad \begin{aligned} -\text{Re}\langle A_{P,L}u, u \rangle &\geq \|u'\|_{L^2(\mathbf{E})}^2 + \text{Re}\langle L\underline{u}, \underline{u} \rangle_{\mathcal{H}} \\ &\geq \|u'\|_{L^2(\mathbf{E})}^2 - \omega C\|u'\|_{L^2(\mathbf{E})}\|u\|_{L^2(\mathbf{E})} \\ &\geq \|u'\|_{L^2(\mathbf{E})}^2 - \omega C \left(\frac{\epsilon}{2}\|u'\|_{L^2(\mathbf{E})}^2 + \frac{1}{2\epsilon}\|u\|_{L^2(\mathbf{E})}^2 \right). \end{aligned}$$

In particular, for $\epsilon = \frac{2}{\omega C}$ we obtain

$$-\text{Re}\langle A_{P,L}u, u \rangle \geq -\frac{\omega^2 C^2}{4}\|u\|_{L^2(\mathbf{E})}^2.$$

This concludes the proof. \square

The restriction of A to $H_0^2(\mathbf{E}_d) \oplus H_0^1(\mathbf{E}_t)$ is denoted by A^0 . The adjoint of A^0 in the Hilbert space $L^2(\mathbf{E})$ is the operator

$$B := \begin{bmatrix} \frac{d^2}{dx^2} & 0 \\ 0 & \frac{d}{dx} \end{bmatrix}, \quad D(B) := H^2(\mathbf{E}_d) \oplus H^1(\mathbf{E}_t).$$

As $A_{P,L}$ is an extension of B^* , $A_{P,L}^*$ is a restriction of B . Therefore it can be described in terms of boundary conditions imposed on B . We introduce the notation

$$\tilde{v} = \begin{bmatrix} \{v_{di}(a_i)\}_{1 \leq i \leq D} \\ \{v_{di}(0)\}_{1 \leq i \leq D} \\ 2^{-\frac{1}{2}} \{(v_{tj}(0) + v_{tj}(a_j))\}_{1 \leq j \leq T} \end{bmatrix} \quad \text{and} \quad \tilde{\tilde{v}} = \begin{bmatrix} \{v'_{di}(a_i)\}_{1 \leq i \leq D} \\ \{-v'_{di}(0)\}_{1 \leq i \leq D} \\ 2^{-\frac{1}{2}} \{(-v_{tj}(0) + v_{tj}(a_j))\}_{1 \leq j \leq T} \end{bmatrix}$$

observing that

$$\tilde{v} = \underline{v}, \quad \text{and} \quad \tilde{\tilde{v}} = J\underline{v}, \quad \text{where} \quad J := \begin{bmatrix} \mathbf{1}_{\mathbb{C}^{2|\mathbf{E}_d|}} & 0 \\ 0 & -\mathbf{1}_{\mathbb{C}^{|\mathbf{E}_t|}} \end{bmatrix}.$$

(The change of sign in the last component is due to the change of the direction on the transport edges).

Lemma 6. *The adjoint operator of $A_{P,L}$ is given the restriction of B onto*

$$D(A_{P,L}^*) := \{(v_d, v_t) \in H^2(\mathbf{E}_d) \oplus H^1(\mathbf{E}_t) \mid (L^* + P)\tilde{v} + P^\perp \tilde{\tilde{v}} = 0\}.$$

Proof. By definition, the adjoint of $A_{P,L}$ is the operator given by

$$\begin{aligned} D(A_{P,L}^*) &:= \{v \in L^2(\mathbf{E}) \mid \exists u \in L^2(\mathbf{E}) \text{ s.t. } \langle A_{P,L} w, v \rangle = \langle w, u \rangle \text{ for all } w \in D(A_{P,L})\}, \\ A_{P,L}^* v &:= u. \end{aligned}$$

To begin with, observe that following the computations in (6) the operator A – without boundary conditions – satisfies

$$\langle Au, v \rangle - \langle u, Bv \rangle = -\langle \underline{u}, \tilde{\tilde{v}} \rangle_{\mathcal{H}} + \langle \underline{u}, \tilde{v} \rangle_{\mathcal{H}}$$

or rather

$$(15) \quad \langle Au, v \rangle - \langle u, Bv \rangle = \left\langle \begin{bmatrix} \underline{u} \\ \underline{u} \end{bmatrix}, \begin{bmatrix} 0 & -\mathbf{1}_{\mathcal{H}} \\ \mathbf{1}_{\mathcal{H}} & 0 \end{bmatrix} \begin{bmatrix} \underline{v} \\ J\underline{v} \end{bmatrix} \right\rangle_{\mathcal{H}^2}, \quad u, v \in H^2(\mathbf{E}_d) \times H^1(\mathbf{E}_t).$$

Recall that $A_{P,L}^*$ is a restriction of the operator B . Hence $v \in D(A_{P,L}^*)$ if and only if the boundary term in (15) vanishes for all $u \in D(A_{P,L})$. The range of

$$[\cdot]_{P,L} : D(A_{P,L}) \rightarrow \mathcal{H}^2, \quad [u]_{P,L} = (\underline{u}, \underline{u})$$

is $\text{Ker}(L + P, P^\perp)$ and hence the boundary term vanishes for a fixed $v \in H^2(\mathbf{E}_d) \times H^1(\mathbf{E}_t)$ and all $u \in D(A_{P,L})$ if and only if

$$(\underline{v}, J\underline{v}) \perp \text{Ker}(-P^\perp, L + P),$$

taking into account that

$$\begin{bmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{bmatrix} \text{Ker}(L + P, P^\perp) = \text{Ker}(-P^\perp, L + P).$$

Since the orthogonal complement of the space $\text{Ker}(-P^\perp, L + P)$ is exactly $\text{Ker}(L^* + P, P^\perp)$ one summarizes that $v \in D(A_{P,L}^*)$ if and only if $v \in H^2(\mathbf{E}_d) \times H^1(\mathbf{E}_t)$ and

$$(\underline{v}, J\underline{v}) = (\tilde{v}, \tilde{\tilde{v}}) \in \text{Ker}(L^* + P, P^\perp).$$

This completes the proof. \square

Proof of Theorem 4. It is known ([10, Cor. II.3.17]) that a sufficient condition for a densely defined operator to have m -dissipative closure is that both it and its adjoint are dissipative. By Lemma 5 $A_{P,L}$ is quasi-dissipative for any L and dissipative whenever $-L$ is dissipative. Like in Lemma 5 one proves that conversely the operator $A_{P,L}^*$ is quasi-dissipative for any choice of L and dissipative whenever $-L$ is dissipative.

To conclude the proof it suffices to check that $A_{P,L}$ is actually closed. Because both the first and the second derivative without boundary conditions are closed operators, in our case it suffices to check that the boundary conditions are respected in the limit. This follows from the fact that the operators $u \mapsto \underline{u}$ and $u \mapsto \underline{\underline{u}}$ are bounded from $H^2(\mathbf{E}_d) \oplus H^1(\mathbf{E}_t)$ to \mathcal{H} . \square

Remark 7. Observe that dissipativity of the matrix $-L$ is sufficient but not necessary for $A_{P,L}$ to be m -dissipative. By (14) one obtains the estimate

$$\operatorname{Re}\langle A_{P,L}u, u \rangle \leq -\|u'\|_{L^2(\mathbf{E})}^2 + \omega C \left(\frac{\epsilon}{2} \|u'\|_{L^2(\mathbf{E})}^2 + \frac{1}{2\epsilon} \|u\|_{L^2(\mathbf{E})}^2 \right) \quad \text{for all } u \in D(A_{P,L}),$$

for some $C > 0$ only depending on the total length of the graph and all $\epsilon > 0$.

To give a concrete example of an m -dissipative operator $A_{P,L}$ where $-L$ is not dissipative we consider the graph consisting of one transport and one diffusion edge with length $a_{1D} = a_{1T} = l/2$, for some $l > 0$. We consider boundary conditions as in (3) by taking

$$P := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2^{-1} & 2^{-1} \\ 0 & 2^{-1} & 2^{-1} \end{bmatrix} \quad \text{and} \quad L_C := -\frac{1}{C}P^\perp,$$

where $C > 0$ is equal the constant appearing in the above estimate. We take advantage of the degrees of freedom that are left: Set $\omega := \|L_C\| = C^{-1}$, and plugging $\epsilon = 1$ in the above inequality we obtain

$$\operatorname{Re}\langle A_{P,L}u, u \rangle \leq -\frac{1}{2}\|u'\|_{L^2(\mathbf{E})}^2 + \frac{1}{2}\|u\|_{L^2(\mathbf{E})}^2 \quad \text{for all } u \in D(A_{P,L_C}).$$

Since P defines a Dirichlet boundary condition on one endpoint of \mathbf{E}_d , by the one-dimensional Poincaré inequality [3, Satz 5.16] there exists an $\alpha > 0$, independent of l , such that ¹

$$\|u'\|_{L^2(\mathbf{E})}^2 \geq \frac{2\alpha^2}{l^2} \|u\|_{L^2(\mathbf{E})}^2 \quad \text{for all } u \in D(A_{P,L_C}).$$

Therefore if $l > \alpha$

$$\operatorname{Re}\langle A_{P,L}u, u \rangle \leq \left(\frac{\alpha^2}{l^2} - \frac{1}{2} \right) \|u\|_{L^2(\mathbf{E})}^2 \leq 0,$$

i.e., A_{P,L_C} is dissipative even if the rank one operator $-L_C = \frac{1}{C}P^\perp$ was not.

Corollary 8. Let $-L$ be dissipative. If additionally the matrix semigroup generated by $-L$ on \mathcal{H} is contractive with respect to the ∞ -norm, then the part of $A_{P,L}$ in $L^p(\mathbf{E})$ generates a semigroup of contractions in $L^\infty(\mathbf{E})$ for each $p \in [2, \infty]$, which is strongly-continuous for $p < \infty$.

If the matrix semigroup generated by L^* on \mathcal{H} is contractive with respect to the ∞ -norm, then the semigroup generated by $A_{P,L}$ in $L^2(\mathbf{E})$ extrapolates to a strongly-continuous semigroup of contractions in $L^p(\mathbf{E})$ for each $p \in [1, 2)$.

Recall that the semigroup $(e^{tA})_{t \geq 0}$ generated by an $n \times n$ matrix $K = (k_{ih})$ with complex-valued coefficients is ∞ -contractive if and only if

$$(16) \quad \operatorname{Re} k_{ii} + \sum_{h \neq i} |k_{ih}| \leq 0 \quad \text{for all } i = 1, \dots, n,$$

¹ Observe that functions in $D(A_{P,L_C})$ are in general not of class $H^2(0, l)$ (in fact, not even $H^1(0, l)$), but this is not relevant: in order to apply Poincaré's inequality it suffices to have a function that is a.e. weakly differentiable, and the possibility to find a path from each point of the graph to the endpoint(s) where the function vanishes; and that the boundary values are uniquely determined along this path – this follows in our case from the fact that $u_t(0)$ and $u_t(a_t)$ are uniquely determined, since the system

$$u_t(0) + u_t(a_t) = \sqrt{2}u_d(0) \quad \text{and} \quad -u_t(0) + u_t(a_t) = \sqrt{2}u_d'(0)$$

admits a unique solution for all $u_d(0), u_d'(0)$.

cf. [18, Lemma 6.1].

The proof of this result is based on a generalization due to Yokota of Brezis' classical results for invariance of closed convex sets of a Hilbert space under the semigroup generated by a subdifferential. In the linear case, his results read as follows, cf. [25, Thm. 2.4].

Lemma 9. *Let X be a complex Hilbert space and $K \subset X$ be closed and convex, and denote by P_K the orthogonal projector onto K . Let $T - \omega$ be an m -dissipative operator for some $\omega \geq 0$ and $(S(t))_{t \geq 0}$ be the strongly-continuous semigroup generated by T . Then K is invariant under $(S(t))_{t \geq 0}$ if and only if*

$$\operatorname{Re}\langle Tu, u - P_K u \rangle \leq \omega \|u - P_K u\|^2 \quad \text{for all } u \in D(T).$$

Proof of Corollary 8. Let K be the unit ball of $L^\infty(\mathbf{E})$. The associated orthogonal projector is given by

$$P_K u := (|u| \wedge 1) \operatorname{sgn} u \quad \text{and therefore} \quad u - P_K u := (|u| - 1)^+ \operatorname{sgn} u, \quad u \in L^2(\mathbf{E}).$$

Accordingly,

$$(P_K u)' := u' \mathbf{1}_{\{|u| \leq 1\}} \quad \text{and} \quad (u - P_K u)' := u' \mathbf{1}_{\{|u| > 1\}}, \quad u \in H^1(\mathbf{E}).$$

Let us study the condition in Lemma 9, which in our case reduces to

$$\operatorname{Re}\langle A_{P,L} u, u - P_K u \rangle \leq 0 \quad \text{for all } u \in D(A_{P,L}).$$

Writing with an abuse of notation $P_K u = (P_K u_d, P_K u_t)$ (this is not completely inconsistent, due to locality of P_K), one has for all $u \in H^1(\mathbf{E})$

$$\begin{aligned} -\operatorname{Re} \int_{\mathbf{E}_d} \langle u_d'', (u_d - P_K u_d) \rangle &= -\operatorname{Re}[u_d', (u_d - P_K u_d)']_{\partial \mathbf{E}_d} + \operatorname{Re} \int_{\mathbf{E}_d} \langle u_d', (u_d - P_K u_d)' \rangle \\ &= -\operatorname{Re}[u_d', (u_d - P_K u_d)']_{\partial \mathbf{E}_d} \\ &\quad + \operatorname{Re} \int_{\mathbf{E}_d} \langle (P_K u_d)', (u_d - P_K u_d)' \rangle + \operatorname{Re} \int_{\mathbf{E}_d} \langle (u_d - P_K u_d)', (u_d - P_K u_d)' \rangle \\ &= -\operatorname{Re}[u_d', (u_d - P_K u_d)']_{\partial \mathbf{E}_d} + \int_{\mathbf{E}_d} \|(u_d - P_K u_d)'\|^2, \end{aligned}$$

and likewise

$$\begin{aligned} \operatorname{Re} \int_{\mathbf{E}_t} \langle u_t', (u_t - P_K u_t) \rangle &= \operatorname{Re} \int_{\mathbf{E}_d} \langle (P_K u_t)', (u_t - P_K u_t) \rangle + \operatorname{Re} \int_{\mathbf{E}_d} \langle (u_t - P_K u_t)', (u_t - P_K u_t) \rangle \\ &= \operatorname{Re} \int_{\mathbf{E}_t} \|(u_t - P_K u_t)\|^2 - \operatorname{Re} \int_{\mathbf{E}_t} \langle u_t', (u_t - P_K u_t) \rangle, \end{aligned}$$

whence

$$\operatorname{Re} \int_{\mathbf{E}_t} \langle u_t', (u_t - P_K u_t) \rangle = \frac{1}{2} \int_{\mathbf{E}_t} \|(u_t - P_K u_t)\|^2.$$

(Here each disappearance of an integral terms follows from the fact that the integrand is the product of two functions with disjoint support). We conclude that for all $u \in D(A_{P,L})$

$$\operatorname{Re}\langle A_{P,L} u, u - P_K u \rangle = - \int_{\mathbf{E}_d} \|(u_d - P_K u_d)'\|^2 - \operatorname{Re}\langle L(\underline{u} - P_K \underline{u}), (\underline{u} - P_K \underline{u}) \rangle_{\mathcal{H}} \leq 0,$$

where the last inequality follows from dissipativity of $-L$. Hence, under our assumptions the semigroup generated by $A_{P,L}$ is both $L^2(\mathbf{E})$ - and $L^\infty(\mathbf{E})$ -contractive. By the Riesz–Thorin interpolation theorem, each semigroup operator $e^{tA_{P,L}}$ extends to a bounded (in fact, contractive) linear operator on $L^p(\mathbf{E})$, for all $p \in [2, \infty]$. Strong continuity for all $p < \infty$ is also clear. The second assertion can be proved by duality, taking into account Lemma 6. Strong continuity of the semigroup in $L^1(\mathbf{E})$ is not obvious, but is a consequence of [23, Prop. 5]. In fact, by Lemma 12 below $A_{P,L}$ has compact resolvent and therefore by [10, Cor. 2.15] each orbit of the generated semigroup is relatively compact, hence weakly relatively compact. \square

Remark 10. *Instead of considering the transport-diffusion-type Cauchy problem associated with dissipative operators, one might think of a Schrödinger-type Cauchy problem involving self-adjoint operators with mixed dynamics. To this aim, consider the symmetric operator*

$$S^0 := \begin{bmatrix} \frac{d^2}{dx^2} & 0 \\ 0 & i \frac{d}{dx} \end{bmatrix}, \quad D(S^0) := H_0^2(\mathbf{E}_d) \oplus H_0^1(\mathbf{E}_t).$$

It has equal deficiency indices $(2|\mathbf{E}_d| + |\mathbf{E}_t|, 2|\mathbf{E}_d| + |\mathbf{E}_t|)$ and its adjoint $S = (S^0)^$ is formally the same operator with domain $H^2(\mathbf{E}_d) \oplus H^1(\mathbf{E}_t)$. Hence there exists self-adjoint extensions and these can be parametrized in terms of boundary conditions. One defines the appropriately modified vectors of boundary values*

$$\bar{u} := \begin{bmatrix} \{u_{di}(a_{di})\}_{1 \leq i \leq D} \\ \{u_{di}(0)\}_{1 \leq i \leq D} \\ 2^{-\frac{1}{2}} \{u_{tj}(a_{tj}) + u_{tj}(0)\}_{1 \leq j \leq T} \end{bmatrix} \quad \text{and} \quad \bar{\bar{u}} := \begin{bmatrix} \{u'_{di}(a_{di})\}_{1 \leq i \leq D} \\ \{-u'_{di}(0)\}_{1 \leq i \leq D} \\ i \cdot 2^{-\frac{1}{2}} \{-u_{tj}(a_{tj}) + u_{tj}(0)\}_{1 \leq j \leq T} \end{bmatrix}$$

to obtain the well known Hermite symplectic form on the space of boundary values

$$\langle Su, v \rangle - \langle u, Sv \rangle = \left\langle \begin{bmatrix} \bar{u} \\ \bar{\bar{u}} \end{bmatrix}, \begin{bmatrix} 0 & -\mathbb{1}_{\mathcal{H}} \\ \mathbb{1}_{\mathcal{H}} & 0 \end{bmatrix} \begin{bmatrix} \bar{v} \\ \bar{\bar{v}} \end{bmatrix} \right\rangle_{\mathcal{H}^2}, \quad u, v \in H^2(\mathbf{E}_d) \oplus H^1(\mathbf{E}_t).$$

It is known that there is a one-to-one correspondence between the self-adjoint extensions of symmetric operators and the maximal isotropic subspaces with respect to this Hermite symplectic form. A unique parametrization of such a subspace is given in terms of a projection P and a Hermitian operator L acting in $\text{Ker} P$. Therefore any self-adjoint realization $S_{P,L}$ of S^0 is a restriction of S onto a domain of the type

$$D(S_{P,L}) = \{u \in H^2(\mathbf{E}_d) \oplus H^1(\mathbf{E}_t) \mid P\bar{u} = 0 \text{ and } L\bar{u} + P^\perp \bar{\bar{u}} = 0\}.$$

The spectrum of the self-adjoint operator $S_{P,L}$ is purely discrete and there are sequences of eigenvalues going to $+\infty$ as well as to $-\infty$. These self-adjoint operators can be interpreted as Hamiltonian consisting of a standard Laplacian and a less usual moment-type observable. As already mentioned, moment operators on graphs have been recently studied in [11]. By Stone's theorem, for self-adjoint $S_{P,L}$ the Cauchy problem

$$\begin{cases} (i \frac{\partial}{\partial t} - S_{P,L}) u(x, t) = 0, & t \in \mathbb{R}, \\ u(\cdot, 0) = u_0 \end{cases}$$

is governed by a unitary group.

3. POSITIVITY

Observe that $L^2(\mathbf{E})$ is a Hilbert lattice, hence we can discuss positivity of the semigroup.

Theorem 11. *Let P an orthogonal projector in \mathcal{H} and L a $(2|\mathbf{E}_d| \times |\mathbf{E}_t|) \times (2|\mathbf{E}_d| \times |\mathbf{E}_t|)$ -matrix such that $L = P^\perp L P^\perp$, where $P^\perp = \text{Id} - P$. Then the following assertions hold.*

- (a) *The semigroup generated by $A_{P,L}$ leaves the set of real-valued functions invariant if and only if L has real entries.*
- (b) *The semigroup generated by $A_{P,L}$ is positive if and only if L has real entries that are positive off-diagonal.*

Proof. (a) By Lemma 9 and reasoning as in the proof of [20, Prop. 2.5], one sees that the semigroup generated by $A_{P,L}$ is real if and only if $(A_{P,L} \text{Re } u, \text{Im } u) \in \mathbb{R}$ for all $u \in D(A_{P,L})$. Taking into account (6), a direct computation shows the assertion.

(b) By Proposition 5, $A_{P,L}$ is always quasi-dissipative, say with constant ω . By [19, Thm. C-II.1.2] it suffices to show that our assumptions on L are satisfied if and only if $A_{P,L} - \omega$ is dispersive. However, because the semigroup generated by $A_{P,L} - \omega$ is clearly positive if and only if so is the semigroup generated by $A_{P,L}$, we can confine ourselves to the case of $A_{P,L}$ dissipative. In other words, it suffices to check that our assumptions on L are satisfied if and only if for every $u \in D(A_{P,L})$ – in fact, by (a), if for every real-valued $u \in D(A_{P,L})$ – there exists $0 \leq \phi_u \in L^2(\mathbf{E})$ such that

- $\|\phi_u\|_{L^2(\mathbf{E})} \leq 1$,
- $\langle u, \phi_u \rangle_{L^2(\mathbf{E})} = \|u^+\|_{L^2(\mathbf{E})}$ and
- $\langle A_{P,L} u, \phi_u \rangle_{L^2(\mathbf{E})} \leq 0$.

Let in fact $u \in D(A_{P,L})$ be real-valued and define ϕ_u as a vector in the positive cone of $L^2(\mathbb{E})$ by

$$\phi_u := \begin{bmatrix} \frac{u_d^+}{\|u^+\|_{L^2(\mathbb{E})}} \\ \frac{u_t^+}{\|u^+\|_{L^2(\mathbb{E})}} \end{bmatrix}.$$

Then, one has

$$\|\phi_u\|_{L^2(\mathbb{E})}^2 = \frac{1}{\|u^+\|_{L^2(\mathbb{E})}^2} \left(\int_{\mathbb{E}_d} |u_d^+|^2 + \int_{\mathbb{E}_t} |u_t^+|^2 \right) = 1.$$

Furthermore,

$$\begin{aligned} \langle u, \phi_u \rangle_{L^2(\mathbb{E})} &= \frac{1}{\|u^+\|_{L^2(\mathbb{E})}} \left(\int_{\mathbb{E}_d} \langle u_d, u_d^+ \rangle + \int_{\mathbb{E}_t} \langle u_t, u_t^+ \rangle \right) \\ &= \frac{1}{\|u^+\|_{L^2(\mathbb{E})}} \left(\int_{\mathbb{E}_d} |u_d^+|^2 + \int_{\mathbb{E}_t} |u_t^+|^2 \right) \\ &= \|u^+\|_{L^2(\mathbb{E})}. \end{aligned}$$

Finally, we take a closer look at (6) and observe that

$$\begin{aligned} - \int_{\mathbb{E}_t} \langle u'_t, u_t \rangle \mathbb{1}_{\{u_t \geq 0\}} &= - \int_{\mathbb{E}_t} \langle u'_t, u_t^+ \rangle \\ &= - \langle u_t, u_t^+ \rangle + \int_{\mathbb{E}_t} \langle u_t, (u_t^+)' \rangle \\ &= - \langle u_t, u_t^+ \rangle_{\partial \mathbb{E}_t} + \int_{\mathbb{E}_t} \langle u_t, u'_t \rangle \mathbb{1}_{\{u_t \geq 0\}}, \end{aligned}$$

whence

$$\begin{aligned} \|u^+\|_{L^2(\mathbb{E})} \langle A_{P,L} u, \phi_u \rangle &= \int_{\mathbb{E}_d} \langle u''_d, u_d^+ \rangle - \int_{\mathbb{E}_t} \langle u'_t, v_t \rangle \\ &= - \int_{\mathbb{E}_d} \|u'_d\|_{L^2(\mathbb{E}_d)}^2 \mathbb{1}_{\{u_d \geq 0\}} + \langle u'_d, u_d^+ \rangle_{\partial \mathbb{E}_d} - \frac{1}{2} \langle u_t, u_t^+ \rangle_{\partial \mathbb{E}_t} \\ &= - \int_{\mathbb{E}_d} \|u'_d\|_{L^2(\mathbb{E}_d)}^2 \mathbb{1}_{\{u_d \geq 0\}} + \langle \underline{u}, \underline{u}^+ \rangle_{\mathbb{C}^{2|\mathbb{E}_d| \times |\mathbb{E}_t|}} \\ &= - \int_{\mathbb{E}_d} \|u'_d\|_{L^2(\mathbb{E}_d)}^2 \mathbb{1}_{\{u_d \geq 0\}} - \langle L \underline{u}, \underline{u}^+ \rangle_{\mathbb{C}^{2|\mathbb{E}_d| \times |\mathbb{E}_t|}}. \end{aligned}$$

Since the boundary values of u and u' that appear in \underline{u} are mutually independent, one concludes that $\langle A_{P,L} u, \phi_u \rangle \leq 0$ if and only if

$$(17) \quad \langle L \xi, \xi^+ \rangle_{\mathbb{R}^{2|\mathbb{E}_d| \times |\mathbb{E}_t|}} \geq 0 \quad \text{for all } \xi \in \mathbb{R}^{2|\mathbb{E}_d| \times |\mathbb{E}_t|}.$$

Because ξ^+ is the orthogonal projection of ξ onto the positive cone of $\mathbb{R}^{2|\mathbb{E}_d| \times |\mathbb{E}_t|}$ and $\langle L \cdot, \cdot \rangle$ is the quadratic form associated with L , we deduce from the invariance criterion [20, Thm. 2.2] that (17) is satisfied if and only if the semigroup generated by L is positive, i.e., if and only if L has real entries that are positive off-diagonal. \square

We close this section by formulating a conjecture on the general behavior of the semigroups generated by the m-dissipative operators $A_{P,L}$.

Conjecture 1. *Let $\mathbb{E}_t \neq \emptyset$. If a function f is supported in $\mathbf{e} \in \mathbb{E}_t$, then the semigroup generated by $A_{P,L}$ will shift its profile until the support of $e^{tA_{P,L}} f$ hits an endpoint of \mathbf{e} . Because $e^{tA_{P,L}} f$ has in this lapse of time the same profile of f , the semigroup cannot be immediately smoothing. In particular, it cannot be analytic – in fact, not even immediately differentiable. On the other hand, it seems reasonable to imagine that the semigroup smoothens the profile of a function as soon as it reaches an edge in \mathbb{E}_d . We conjecture that if $\mathbb{E}_d \neq \emptyset$, then the semigroup is differentiable for all $t > T$, where T is the length of the longest path inside \mathbb{E}_t (to compute taking into account the possibly coupled boundary conditions).*

4. SPECTRAL THEORY

Taking into account Lemma 3, we promptly obtain the following.

Lemma 12. *For all orthogonal projectors P in \mathcal{H} and all linear operators L acting in $\text{Ker}P$, the operators $A_{P,L}$ have resolvent of p -th Schatten class for all $p > 1$ (and, in particular, of Hilbert–Schmidt class). In particular, $A_{P,L}$ has only pure point spectrum.*

4.1. Non-zero eigenvalues. In order to determine the pure point spectrum of $A_{P,L}$, a natural *Ansatz* for finding eigenfunctions is to take $k \in \mathbb{C} \setminus \{0\}$ and to consider

$$\phi(x, k) = \begin{cases} \alpha_{di}(k)e^{ikx} + \beta_{di}(k)e^{-ikx}, & x \in \mathbf{e}_{di}, i = 1, \dots, D, \\ \gamma_{tj}(k)e^{k^2x}, & x \in \mathbf{e}_{tj}, j = 1, \dots, T. \end{cases}$$

The boundary conditions $(P + L)\phi(\cdot, k) + P^\perp \phi(\cdot, k) = 0$ are encoded into

$$[(P + L)X(k) + P^\perp Y(k)] \begin{bmatrix} \alpha_d(k) \\ \beta_d(k) \\ \gamma_t(k) \end{bmatrix} = 0,$$

where $\{\alpha_d(k)\}_{i=1, \dots, D} = \alpha_{di}(k)$, $\{\beta_d(k)\}_{i=1, \dots, D} = \beta_{di}(k)$, $\{\gamma_t(k)\}_{j=1, \dots, T} = \gamma_{tj}(k)$ are the sought after coefficients. The matrices

$$X(k) = \begin{bmatrix} e^{ik\mathbf{a}_d} & e^{-ik\mathbf{a}_d} & 0 \\ \mathbb{1} & \mathbb{1} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}}(1 + e^{k^2\mathbf{a}_t}) \end{bmatrix},$$

$$Y(k) = \begin{bmatrix} ik e^{ik\mathbf{a}_d} & -ik e^{-ik\mathbf{a}_d} & 0 \\ -ik & ik & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}}(1 - e^{k^2\mathbf{a}_t}) \end{bmatrix}$$

act in \mathcal{H} are given with respect to the decomposition $\mathcal{H} = \mathcal{H}_d^+ \oplus \mathcal{H}_d^- \oplus \mathcal{H}_t$. Here the notation

$$\{e^{\pm k^2\mathbf{a}_t}\}_{j,l=1, \dots, T} = \delta_{jl}e^{\pm k^2\mathbf{a}_{tj}} \quad \text{and} \quad \{e^{\pm ik\mathbf{a}_d}\}_{j,l=1, \dots, D} = \delta_{jl}e^{\pm ik\mathbf{a}_{dj}}$$

is used. Accordingly, the following holds.

Proposition 13. *For all orthogonal projectors P in \mathcal{H} and all linear operators L acting in $\text{Ker}P$, the number $-k^2 \in \mathbb{C} \setminus \{0\}$ is an eigenvalue of $A_{P,L}$ if and only if the matrix*

$$Z(k) := [(P + L)X(k) + P^\perp Y(k)],$$

has non trivial null space. The geometric multiplicity of $-k^2$ equals the dimension of $\text{Ker}Z(k)$.

Hence, the secular equation is

$$\det Z(k) = 0.$$

Example 14. *Consider the graph consisting of one diffusion edge of length a_D and one transport edge of length a_T . Let P be as in Remark 7,*

$$P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2^{-1} & 2^{-1} \\ 0 & 2^{-1} & 2^{-1} \end{bmatrix} \quad \text{and} \quad L = 0.$$

Then the operator $A_{P,L}$ is m -dissipative and the secular equation becomes

$$\det Z(k) = \frac{i}{\sqrt{2}} \left[\sin(ka_D) \left(1 - e^{k^2\mathbf{a}_t} \right) + k \cos(ka_D) \left(1 + e^{k^2\mathbf{a}_t} \right) \right] = 0.$$

In particular the spectrum of $A_{P,L}$ contains a sequence of real eigenvalues going to $-\infty$.

It seems in general difficult to give precise statements on the distribution of the eigenvalues.

4.2. Eigenvalue zero. For the eigenvalue zero one uses for the eigenfunctions the *Ansatz*

$$\phi_0(x) = \begin{cases} \alpha_{di}(0) + \beta_{di}(0)x, & x \in \mathbf{e}_{di}, i = 1, \dots, D, \\ \gamma_{tj}(0), & x \in \mathbf{e}_{tj}, j = 1, \dots, T. \end{cases}$$

The boundary conditions $(P + L)\phi(\cdot, 0) + P^\perp \phi(\cdot, 0) = 0$ are encoded into

$$[(L + P)X_0 + P^\perp Y_0] \begin{bmatrix} \alpha_d(0) \\ \beta_d(0) \\ \gamma_t(0) \end{bmatrix} = 0$$

with

$$X_0 = \begin{bmatrix} \mathbb{1} & \mathbf{a}_d & 0 \\ \mathbb{1} & 0 & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} \quad \text{and} \quad Y_0 = \begin{bmatrix} 0 & \mathbb{1} & 0 \\ 0 & -\mathbb{1} & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

where $\{\mathbf{a}_d\}_{j,l=1,\dots,D} = \delta_{jl}a_{dj}$. Hence we obtain a characterization for the eigenvalue zero.

Proposition 15. *For all orthogonal projectors P in \mathcal{H} and all linear operators L acting in $\text{Ker}P$, the operator $A_{P,L}$ is invertible if and only if*

$$\det Z_0 \neq 0, \quad \text{where} \quad Z_0 = (P + L)X_0 + P^\perp Y_0.$$

In particular the invertibility of the operator $A_{P,L}$ is independent of the lengths of the transport edges.

Example 16. *Consider again the graph given in Example 14 and let P be the projector given in Example 14 and Remark 7. Let be $L_C = CP^\perp$, where $P^\perp = \text{Id} - P$ and for arbitrary $C \in \mathbb{C}$. Then*

$$\det Z_0 = -2^{-\frac{1}{2}} - Ca_D 2^{\frac{1}{2}}$$

and therefore A_{P,L_C} is invertible only for $C \neq -(2a_D)^{-1}$.

4.3. The resolvent operator. Knowing the resolvent $R(\lambda, A_{P,L}) = (A_{P,L} - \lambda)^{-1}$ for $A_{P,L}$ dissipative and for λ in the right halfplane, one can describe the semigroup generated by $A_{P,L}$ by means of the inverse Laplace transform as

$$(18) \quad e^{tA_{P,L}}u = \lim_{n \rightarrow \infty} \int_{\varepsilon - in}^{\varepsilon + in} e^{t\lambda} R(\lambda, A_{P,L})u \, d\lambda, \quad u \in L^2(\mathbf{E}_d) \times L^2(\mathbf{E}_t),$$

for any $\varepsilon > 0$, see [2, Thm. 3.12.2]. In fact, in the following an explicit formula for the resolvent is given in terms of the boundary conditions and the edge lengths. First we define the shorthand notation

$$\int_{\mathbf{G}} u := \sum_{i \in \mathbf{E}_d} \int_0^{a_{di}} u_{di}(x) dx + \sum_{j \in \mathbf{E}_t} \int_0^{a_{tj}} u_{tj}(x) dx, \quad \text{for } u \in L^2(\mathbf{G}).$$

Proposition 17. *For all orthogonal projectors P in \mathcal{H} , all linear operators L acting in $\text{Ker}P$ and for all $k \neq 0$ such that $-k^2 \in \rho(A_{P,L})$, the resolvent operator $R(k) = (A_{P,L} + k^2)^{-1}$ is the integral operator given by*

$$R(k)u(x) := \int_{\mathbf{G}} r(x, \cdot, k)u(\cdot)$$

with kernel

$$r(x, y, k) := \{r_0(x, y, k) - \Phi(x, k)\Sigma(P, L, k)\Psi(y, k)\} W(k).$$

Here we have denoted

$$\Sigma(P, L, k) := [(P + L)X(k) + P^\perp Y(k)]^{-1}[P^\perp R_1(k) + (L + P)R_2(k)]$$

and furthermore

$$\begin{aligned} r_0(x, y, k) &:= \begin{bmatrix} r_d(x, y, k) & 0 \\ 0 & r_t(x, y, k^2) \end{bmatrix}, \\ W(k) &:= \begin{bmatrix} \frac{i}{2k} \mathbb{1}_{\mathbb{C}^{|\mathbb{E}_d|}} & 0 \\ 0 & \mathbb{1}_{\mathbb{C}^{|\mathbb{E}_t|}} \end{bmatrix}, \\ \{r_d(x, y, k)\}_{n,m} &:= \delta_{n,m} e^{ik|x-y|}, \quad n, m = 1, \dots, D, \\ \{r_t(x, y, k)\}_{j,l} &:= \delta_{j,l} \begin{pmatrix} e^{k^2(x-y)}, & x < y \\ 0, & x \geq y \end{pmatrix}, \quad j, l = 1, \dots, T. \end{aligned}$$

Finally,

$$\Phi(x, k) := \begin{bmatrix} e^{ikx} & e^{-ikx} & 0 \\ 0 & 0 & e^{k^2x} \end{bmatrix}, \quad \Psi(x, k) := \begin{bmatrix} e^{iky} & 0 \\ e^{-iky} & 0 \\ 0 & e^{-k^2y} \end{bmatrix},$$

where the entries are diagonal matrices whose entries are functions with arguments from the corresponding edges and

$$R_1(k) := \begin{bmatrix} ik \mathbb{1}_{\mathbb{C}^{|\mathbb{E}_d|}} & 0 & 0 \\ 0 & ik e^{ik\mathbb{a}_d} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} \mathbb{1}_{\mathbb{C}^{|\mathbb{E}_t|}} \end{bmatrix}, \quad R_2(k) := \begin{bmatrix} \mathbb{1}_{\mathbb{C}^{|\mathbb{E}_d|}} & 0 & 0 \\ 0 & e^{ik\mathbb{a}_d} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} \mathbb{1}_{\mathbb{C}^{|\mathbb{E}_t|}} \end{bmatrix}.$$

Proof. It is sufficient to prove that $r(x, y, k)$ is the Green's function of the operator $(A_{P,L} + k^2)$. Consider the unperturbed operator

$$R_0(k)u(x) = \int_{\mathbb{G}} r_0(x, \cdot, k)W(k)u(\cdot) \quad \text{for } u \in \left(\bigoplus_{i=1}^D C_0^\infty([0, a_{di}]) \bigoplus_{j=1}^T C_0^\infty([0, a_{tj}]) \right).$$

The equation $(A + k^2)R_0(k)u = u$ is satisfied on the diffusion edges as $\frac{i}{2k}e^{ik|x-y|}$ is the Green's function of $L_d(k) = \frac{d^2}{dx^2} - k^2$ on the whole real line (this follows from standard arguments using the Fourier transform). By continuing functions $u_i \in L^2([0, a_{di}])$ trivially onto the real line the claim follows. Similarly the diagonal entries of $r_t(x, y, k)$ are the Green's function for $L_t(k) = -\frac{d}{dx} - k^2$ on the whole real line, which follows from standard arguments from the theory of ordinary differential equations. Again by continuing functions u_j in $L^2([0, a_{tj}])$ trivially onto the real line the claim follows. For the correction term one has

$$(A + k^2) \int_{\mathbb{G}} \Phi(x, k) \Sigma(P, L, k) \Psi(\cdot, k) u(\cdot) = 0.$$

Therefore $(A + k^2)R(k)u = u$. As $\left(\bigoplus_{i=1}^D C_0^\infty([0, a_{di}]) \bigoplus_{j=1}^T C_0^\infty([0, a_{tj}]) \right)$ is dense in $L^2(\mathbb{G})$ and $r(\cdot, \cdot, k)$ defines for all $k \neq 0$ such that $-k^2 \in \rho(A_{P,L})$ a bounded linear operator on $L^2(\mathbb{G} \times \mathbb{G})$. One concludes by density that $(A + k^2)R(k)u = u$ for all $u \in L^2(\mathbb{G})$.

It remains to prove that $R(k)u \in D(A_{P,L})$. Observe that for all $a > 0$ and all $u \in L^2(0, a)$

$$\begin{aligned} \left[\int_0^a e^{ik|x-y|} u(y) dy \right]_{x=0} &= \int_0^a e^{iky} u(y) dy, \\ \left[\int_0^a e^{ik|x-y|} u(y) dy \right]_{x=a} &= e^{ika} \int_0^a e^{-iky} u(y) dy, \\ \left[-\frac{d}{dx} \int_0^a e^{ik|x-y|} u(y) dy \right]_{x=0} &= ik \int_0^a e^{iky} u(y) dy, \\ \left[\frac{d}{dx} \int_0^a e^{ik|x-y|} u(y) dy \right]_{x=a} &= ik e^{ika} \int_0^a e^{-iky} u(y) dy, \end{aligned}$$

and considering only the edge $[0, a]$

$$\begin{aligned} \left[\int_0^a r_t(x, y, k^2) u(y) dy \right]_{x=0} &= \int_0^a e^{-k^2 y} f(y) dy, \\ \left[\int_0^a r_t(x, y, k^2) u(y) dy \right]_{x=a} &= 0. \end{aligned}$$

This gives in the matrix notation for $u \in L^2(\mathbf{G})$ and $v \in \mathcal{H}$

$$\begin{aligned} \underline{R_0(k)u(x)} &= R_2(k) \int_{\mathbf{G}} \Psi(k, \cdot) W(k) u(\cdot), & \underline{\Phi(x, k)v} &= X(k)v, \\ \underline{\underline{R_0(k)u(x)}} &= R_1(k) \int_{\mathbf{G}} \Psi(k, \cdot) W(k) u(\cdot), & \underline{\underline{\Phi(x, k)v}}} &= Y(k)v. \end{aligned}$$

Therefore

$$\begin{aligned} \underline{\int_{\mathbf{G}} r(x, \cdot, k) u(\cdot)} &= (R_2(k) - X(k) \Sigma(P, L, k)) \int_{\mathbf{G}} \Psi(\cdot, k) W(k) u(\cdot), \\ \underline{\underline{\int_{\mathbf{G}} r(x, \cdot, k) u(\cdot)}} &= (R_1(k) - Y(k) \Sigma(P, L, k)) \int_{\mathbf{G}} \Psi(\cdot, k) W(k) u(\cdot), \end{aligned}$$

and hence for all $u \in L^2(\mathbf{G})$

$$\underline{\underline{(P + L) \int_{\mathbf{G}} r(x, \cdot, k) f(\cdot) + P^\perp \int_{\mathbf{G}} r(x, \cdot, k) f(\cdot)}} = 0.$$

This proves that $r(\cdot, \cdot, k)$ is the Green's function for the mixed problem. \square

Remark 18. *The statement in Theorem 3.(a) can also be proved also by observing that the kernel $r(\cdot, \cdot, i\kappa)$, $\kappa > 0$ has real coefficients whenever the operator L have real entries. Therefore the resolvents $(A_{P,L} - \kappa^2)^{-1}$ map real-valued functions to real-valued functions for any $\kappa^2 > 0$. Applying the inverse Laplace transform described in (18), one concludes that the semigroup generated by $A_{P,L}$ is real whenever $-L$ is dissipative and real.*

5. DELAYED DIFFUSION EQUATIONS VIA MIXED PDES ON GRAPHS

We conclude this note discussing a possible application of our theory to delayed diffusion equations. It is a classical idea, thoroughly developed e.g. in [5], that delays can be mathematically modeled by means of (auxiliary) transport phenomena. While this theory is classical whenever the delay is “distributed” – i.e., it acts on each point of the domain of diffusion –, it is less standard and technically more involved whenever the delays only concern the boundary values. The situation we want to describe is the following: We consider a ramified structure with an ongoing diffusion process. Incoming particles are absorbed in some nodes and stored there for some time (which depends solely on the features of the node itself), before triggering a flow in the incident edges. This phenomenon can be described by attaching to each such node a fictitious loop, which the particles have to cross before reaching the adjacent edges. A comparable approach has been presented in the recent article [6].

As a tentative motivation of the investigation of this class of problems, we briefly discuss a (much simplified) model of a *dendrodendritic chemical synapse*, referring the reader to any introductory textbook on neuronal modeling (e.g., [22, Chapters 2 and 9] and [8, Chapter 5]) for basic notions and some miscellaneous models, including delayed ones. Also for the sake of simplicity, we drop the absorption term and therefore replace the cable equation usually discussed in theoretical neuroscience by a simpler diffusion equation. (This in fact a bounded perturbation, hence neglectable when it comes to discussing well-posedness). We also remark that our model essentially applies to the case of less exotic axodendritic synapses, if we linearize the active transport phenomena typical of the latter.

Consider two dendrites (modeled by two intervals $\mathbf{e}_1, \mathbf{e}_2$) that are incident in the synapse \mathbf{v} , which is terminal endpoint of \mathbf{e}_1 and initial endpoint of \mathbf{e}_2 . The synaptic input coming from \mathbf{e}_1 undergoes a delay of $\tau_{\text{del}} = 1$ before reaching \mathbf{e}_2 and cannot double back. For the sake of simplicity, we also impose *sealed*

end conditions on the first dendrite \mathbf{e}_1 as well as on the second endpoint of \mathbf{e}_2 , but of course longer chains of neurons may be modeled in a similar way.

The synaptic input is an action potential that lets neurotransmitters be released by synaptic vesicles. Experimental observations suggest that no obvious (linear) algebraic relation exists between the pre- and post-synaptic potential in the dendrites – i.e., between the boundary values of the unknowns u_1, u_2 in the diffusion equations. We propose to discuss this system by a network diffusion problem with boundary delay

$$(BD) \quad \left\{ \begin{array}{lll} \dot{u}_1(t, x) & = & u_1''(t, x), \quad t \geq 0, x \in (0, 1), \\ \dot{u}_2(t, x) & = & u_2''(t, x), \quad t \geq 0, x \in (0, 1), \\ u_1(t, 1) & = & u_1'(t, 1), \quad t \geq 0, \\ -u_2'(t, 0) & = & u_1'(t - 1, 1), \quad t \geq 0, \\ u_1'(t, 0) & = & 0, \quad t \geq 0, \\ u_2'(t, 1) & = & 0, \quad t \geq 0, \\ u_1(0, x) & = & f_1(0, x), \quad x \in (0, 1), \\ u_2(0, x) & = & f_2(0, x), \quad x \in (0, 1), \\ u_1(t, 1) & = & f_{\text{del}}(t), \quad t \in [-1, 0]. \end{array} \right.$$

The first boundary condition, of Robin-type, can be interpreted by saying that part of the reaching the presynaptic nerve terminal is reflected into the entrance dendrite. The second condition is actually the relevant one: It reflects the fact that the conduction speed of the signal in the dendrites is approximatively constant, at least within the same cortical area. In other words, even if the postsynaptic potential will in general have a different amplitude from the presynaptic one, their speed of propagation will be the same. Finally, it is easy to convince ourselves that the above problem is undetermined if the last initial condition on the delay term is not imposed.

In order to implement the delay feature into the node conditions, we introduce an edge \mathbf{e}_{del} and an unknown u_{del} to model the transport of neurotransmitters in the synaptic cleft between the pre- and the postsynaptic neurons, hence effectively introducing a delay phenomenon.

Our aim is now to replace the fourth, delayed equation in (BD) by two node conditions in the endpoints of \mathbf{e}_{del} . More precisely, we impose that

$$u_1'(t, 1) = u_{\text{del}}(t, 0), \quad t \geq 0,$$

as well as

$$-u_2'(t, 0) = u_{\text{del}}(t, 1), \quad t \geq 0.$$

In other words, the flow of postsynaptic potential and the flow of presynaptic potential agree, even if its transmission undergoes a certain delay (which we have normalized).

We are hence led to consider an (undelayed) initial boundary value problem

$$(BD') \quad \left\{ \begin{array}{lll} \dot{u}_1(t, x) & = & u_1''(t, x), \quad t \geq 0, x \in (0, 1), \\ \dot{u}_{\text{del}}(t, x) & = & -u_{\text{del}}'(t, x), \quad t \geq 0, x \in (0, 1), \\ \dot{u}_2(t, x) & = & u_2''(t, x), \quad t \geq 0, x \in (0, 1), \\ u_1'(t, 1) & = & u_{\text{del}}(t, 0), \quad t \geq 0, \\ u_1'(t, 1) & = & u_1(t, 1), \quad t \geq 0, \\ -u_2'(t, 0) & = & u_{\text{del}}(t, 1), \quad t \geq 0, \\ u_1'(t, 0) & = & 0, \quad t \geq 0, \\ u_2'(t, 1) & = & 0, \quad t \geq 0, \\ u_1(0, x) & = & f_1(0, x), \quad x \in (0, 1), \\ u_2(0, x) & = & f_2(0, x), \quad x \in (0, 1), \\ u_{\text{del}}(0, x) & = & f_{\text{del}}(0, x), \quad x \in (0, 1), \end{array} \right.$$

i.e., we have got rid of the boundary delay by passing to the a larger state space. Observe that the above model is intrinsically non-symmetric in the sense that potential can only flow from dendrite \mathbf{e}_1 to \mathbf{e}_2 , but not vice versa. This is a typical feature of *chemical synapses*, as opposed to *electric* ones.

One can check that the problems (BD) and (BD') are equivalent. It should be observed that transport-based synaptic transmission models are not very common in the literature. Due to their numerical and

analytic complexity they are actually often replaced by convective-diffusive (or even purely diffusive) models. A convincing pleading of a transport approach can be found in [24, § 2 and § 6].

To discuss the problem (BD') in our setting, observe that (BD') can be seen as an abstract Cauchy problem on $L^2(\mathbf{E})$ with boundary conditions as in (10), where $|\mathbf{E}_d| = 2$ and $|\mathbf{E}_t| = 1$ with

$$L := \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -\sqrt{2} \\ -\sqrt{2} & 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad P := 0.$$

A direct application of Theorems 4 and 11 yields finally the following.

Proposition 19. *The initial-boundary value problem (BD') is governed by a strongly-continuous semigroup $(T(t))_{t \geq 0}$ on $L^2(\mathbf{E}) = L^2(0, 1) \times L^2(0, 1) \times L^2(0, 1)$. This semigroup is real but non-positive, i.e., there exists t_0 such that $T(t_0)$ is not a positive operator.*

Remark 20. *Observe that the above result does not really depend on our choice to consider a delay interval e_{del} of unit length: we may in fact replace $(0, 1)$ by an interval of arbitrary length. Furthermore, explicite computations show that*

$$\det Z_0 = 0$$

and therefore $A_{P,L}$ is not invertible for any edge lengths. Moreover, $-L$ is not dissipative, hence Theorem 4 cannot be applied to deduce contractivity of the semigroup that governs the problem.

An explanation for the non-positivity of $(T(t))_{t \geq 0}$ comes directly from the biological description of the considered model: Due to lack of physical contact between the presynaptical dendrite and the postsynaptical one, the potential is typically not conserved. This phenomenon has already been observed in [12, § 2] for different transmission conditions.

Remark 21. *More generally one can consider couplings between the transport edge and the two diffusion edges of the form*

$$\begin{aligned} u'_1(t, 1) &= u_{\text{del}}(t, 0), & t \geq 0, \\ u'_1(t, 1) &= \gamma u_1(t, 1), & t \geq 0, \\ -u'_2(t, 0) &= \delta u_2(t, 0) - u_{\text{del}}(t, 1), & t \geq 0. \end{aligned}$$

For any choice of $\gamma, \delta \in \mathbb{R}$ this defines a well-posed problem, since Theorem 4 applies to the system.

We conclude by observing that another possibility – perhaps more natural in certain different contexts – could be to impose transmission of either boundary values at both endpoints. It seems that this setting is not covered by our setting, but we are not able to guess whether this is a hint that such a system is not well-posed.

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